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# Improved Banded Method for Spectral Thermal Radiation in Participating Media with Spectrally Dependent Wall Emittance

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# Abstract

To develop an efficient and practical spectral radiation model for CFD simulations, a banded approach is proposed for a mixture of carbon dioxide and water vapor in varying thermodynamic states. Using a previously reported band dividing scheme, a statistical narrow band model is implemented to provide gray band absorption coefficient databases. The databases were then approximated by certain simple correlations, which can be readily used in CFD calculations of RTE solvers. The correlations were validated in several 1D and 3D benchmarks representing various combustion conditions. The accuracy and CPU cost of the proposed banded approach were studied and compared with those of other similar methods. The results demonstrated that the new approach is an efficient and accurate method that can be conveniently applied in a commercial CFD code for spectral radiation; moreover, it can handle non-gray walls. As a practical case study, the proposed approach was used to simulate radiative heat transfer within a back pass channel of a CFB boiler. The effect of combustion scenarios, i.e., air- and oxygen-fired, boiler load, inlet flow conditions, and wall material, was analyzed by the CFD model. The predictions of two different RTE solvers, i.e., P1 and DO, and the required CPU time were compared for gray and non-gray models.

**Keywords:** Radiation heat transfer, Banded approach, Narrow band calculation, Non-gray gas modeling, Band absorption coefficient, Non-gray wall, Back pass channel, CFB boiler

## **Highlights:**

- An SNB-based banded approach was developed.
- Simple correlations for gray band absorption coefficients were developed.
- The performance of the model was studied in 1D and 3D benchmarks.
- Non-gray wall boundary conditions are best supported by the banded approach.
- A parametric study was conducted for the operational conditions of the back pass channel.

# Nomenclature

<i>a</i> <sub>16</sub>	correlation coefficients in eq. 18 (-)
С	linear scattering phase function coefficient (-)
$E_{b\lambda}$	spectral blackbody emission (W. m <sup>-2</sup> )
G	incident radiation (W. m <sup>-2</sup> )
Ι	radiation intensity (W· sr <sup>-1</sup> )
$\overline{k}$	mean line intensity to line spacing ratio (cm <sup>-1</sup> .atm <sup>-1</sup> )
$k_{\lambda}$	mean absorption coefficient of narrow bands (m <sup>-1</sup> )
l	path length (cm)
L	beam length in definition of optical thickness
т	ordinate direction (-)
M <sub>r</sub>	molar fraction ratio
n	refractive index (-)
$P_t$	total pressure of the mixture (atm)
PL	pressure-path length product (-)
р	gas species partial pressure (atm)
$p_s$	reference pressure (1 bar)
q	radiative heat flux (W. m <sup>-2</sup> )
RST	radiative source term (W. m <sup>-3</sup> )
r	position vector
r <sub>c</sub>	radial distance from centerline in benchmarks (m)
$S_{G}$	additional source of incident radiation (W. m <sup>-2</sup> )
ŝ	solid angle (sr)

Т	gas temperature (K)
$T_c$	temperature of centerline in benchmarks (K)
$T_e$	temperature of exit in benchmarks (K)
$T_s$	reference temperature (298 K)
W <sub>m</sub>	weight of ordinates

# **Greek letters**

extinction coefficient (m <sup>-1</sup> )
average line Lorentz half-width (cm <sup>-1</sup> )
wall emittance (-)
wave number (cm <sup>-1</sup> )
direction cosine
absorption coefficient (m <sup>-1</sup> )
band gray absorption coefficient (m <sup>-1</sup> )
mean line spacing (cm <sup>-1</sup> )
Stefan–Boltzmann constant (5.67×10 <sup>-8</sup> W. m <sup>-2</sup> K <sup>-4</sup> )
scattering coefficient (m <sup>-1</sup> )
transmissivity (-)
wavelength (µm)
wavelengths of band limits (µm)
molar fraction (-)

# Subscripts

b	blackbody
mix	mixture

 $\lambda$  spectral based

w wall

# Abbreviations

CCS	carbon capture and storage
CFB	circulating fluidized bed
CFD	computational fluid dynamics
CHP	convective heating power
DO	discrete ordinate method
FSCK	full spectrum correlated-K method
LBL	line-by-line calculation
NG	non-gray gas model
Oxy	oxygen fired combustion
RT	ray tracing method
RTE	radiative transfer equation
RHP	radiative heating power
SLW	spectral line based weighted sum of gray gas method
SNB	statistical narrow band model
THP	total heating power
WSGG	weighted sum of gray gases model

# Introduction

Numerical modeling of thermal spectral radiation in combustion gases is difficult, as the gas absorption coefficient varies rapidly with wavenumber. The shape and strength of the absorption lines in the spectrum are strongly affected by the thermodynamic state of the gas [1, 2]. Consequently, non-gray gas radiative heat transfer modeling of combustion gases is challenging.

Gray gas models, in which the changes in the absorption coefficient with wavenumber are ignored and an average value is used for the absorption coefficient in the entire spectrum, have been widely used in engineering calculations of combustion systems [3, 4], owing to their simplicity and low computational cost [2]. However, several studies have demonstrated that using gray gas models may often result in significant inaccuracy [1, 5].

Within the part of the electromagnetic wave spectrum where thermal radiation heat transfer occurs, there are a large number of absorption lines forming a histogram for the gas spectral absorption coefficient. The currently available computational resources are insufficient to feasibly include the effect of every individual absorption line in the computational fluid dynamics (CFD) modeling of large-scale combustion systems. Hence, a considerable amount of research has been devoted to developing simplified models to feasibly include the spectral radiation heat transfer of combustion gases in the CFD modeling of large-scale combustors [6, 7, 8, 9, 10]. The line-by-line calculation (LBL) is the most accurate way to account for the spectral radiative properties of molecular gases. In this method, the spectral absorption coefficient in a spectral location is obtained by using the available spectroscopic databases containing a set of spectral line parameters [8]. The gas spectral absorption coefficient varies more with the wavenumber than other quantities. It is the base of the second most accurate spectral model, i.e., the statistical narrow band model (SNB). In this model, the actual profile of the absorption coefficient is replaced by a smoothed averaged profile over narrow bands on the order of 25  $\text{cm}^{-1}$  [2]. The model was originally proposed for atmospheric radiation by Goody [11], but its parameters for high-temperature combustion conditions have been studied later [12, 13]. By analyzing several one-dimensional (1D) benchmarks, Chu et al. [14] reported that the SNB model can be as accurate as LBL. However, owing to their high computational cost, LBL and SNB cannot be used for the modeling of large-scale combustors. Thus, these two methods are currently used to obtain the data required for developing other simpler methods, and to provide benchmark solutions for accuracy evaluation.

In the analysis of practical combustion systems, the total radiative heat flux in the surrounding walls and the radiative source term within the combustion product are the two main objectives. This has urged the development of the so-called global models, which use spectrally integrated radiative properties to calculate the total radiative heat flux and radiative source term. The most widely known models in this category are the weighted sum of gray gases model (WSGG) [15, 16, 17], the full spectrum correlated-K method (FSCK) [18], and the spectral-line-based weighted sum of gray gases method (SLW) [19].

Supporting spectrally dependent radiative properties of surfaces is important in various applications, such as solar receivers [20] and fire detection [21]. A large number of studies have been concerned with measuring and characterizing spectrally dependent wall properties (see for instance [22, 23]); however, this has not yet been implemented in the modeling of the radiative exchange of solar receiver surfaces [24]. To the best of the authors' knowledge, the present study is the first that proposes simple-banded models for including non-gray walls in the CFD simulation of participating media [3, 25].

The information of the spectral location of a certain absorption coefficient is lost in the process of obtaining the global model parameters. Hence, owing to wavelength reordering, global models cannot support spectrally dependent wall emissivity. By contrast, box models are not based on wavenumber reordering and therefore can provide the spectral information of radiative heat transfer. Hence, this study is aimed at providing a simple, fast, and accurate band model that can also support non-gray boundary wall conditions. In banded models (or box models), the radiation heat transfer spectrum is divided into several intervals in which the spectral absorption coefficient is averaged and the gray band absorption coefficient is obtained. The radiative transfer equation is then solved for each interval and the final result is obtained by summing up the results of all the intervals using the associated blackbody fractional function of the intervals as a weighting factor. Owing to the simplicity of the banded approach, its implementation in the overall modeling of combustion systems requires neither a deep understanding of all the details regarding gas spectral radiation heat transfer nor overly large databases, such as those used in SNB [13] or FSCK [18]. Hence, the banded approach can be readily implemented in recent versions of the commercial CFD solver Ansys-Fluent, as the only required information is the band dividing scheme, i.e., the number of bands and band limits, together with the gray band absorption coefficient of each band.

The banded approach is based on the fact that most absorption lines of combustion gases are located in certain regions of the spectrum that are called "bands." Hence, the main challenge in the banded approach is the selection of the optimal bands. Bordbar and Hyppänen [3] have recently used line-by-line spectral profiles of  $CO_2$  and  $H_2O$  in variant thermal conditions and reported an accurate band dividing scheme of 31 bands for the mixture  $H_2O-CO_2$ . Their 31-band solution could provide results as accurate as those by line-by-line integration. However, using 31 bands in the simulation of large-scale systems is computationally expensive and therefore infeasible. In another study, by analyzing the profile of the spectral absorption coefficients of  $H_2O$  and  $CO_2$  in a wide range of thermodynamic states occurring in typical CFB furnaces, Maximov [25] found an optimal band dividing scheme. The bands were identified by

a detailed analysis of certain three-dimensional (3D) benchmarks for air- and oxygen-fired combustion scenarios. This band dividing scheme was also used in the present study.

The purpose of this study is to develop a banded spectral radiation approach and a method that can be applied in practical, fast, and accurate CFD simulations for enclosures with non-gray walls. The aim is to improve the accuracy and CPU cost of the 10-band solution in [25] by deriving more accurate correlations for the bands' gray absorption coefficients. Moreover, the CPU cost of the present 10-band approach is assumed to be significantly less than that of the 31-band solution in [3]. These are demonstrated by accuracy and computational time comparison of several 1D benchmarks. The approach can also handle non-gray walls, which cannot be considered in global models such as WSGG and FSCK. As a practical benefit, the banded model is easy and straightforward to apply in CFD simulation code supporting banded structure in the radiation model (here, Ansys-Fluent). Consequently, the correlations and parameters presented in this study can be readily used in CFD simulations when spectral calculations are required.

Implementing the statistical narrow band method, the gray band absorption coefficient has been obtained for each band. The large dataset of the obtained gray band absorption coefficients was then approximated by certain simple correlations expressing the gray band absorption coefficient as a function of the thermodynamic state of the gas mixture. The correlations, which can be readily used in overall CFD modeling, were validated by 1D and 3D benchmarks [26, 27], and their predictions were compared with those by other banded or global non-gray gas models such as WSGG and FSCK.

As a practical case study, the proposed correlation based banded approach was used to analyze the spectral radiation in a back pass channel of a circulating fluidized bed (CFB) boiler. In CFB combustors, the combustion of fuel particles takes place in a fluidized suspension of ash and other particles. CFB combustion has been widely used for power generation and has several advantages, including fuel flexibility, high combustion performance, and low NOx emissions [1]. Owing to the increasing attention given to new carbon capture and storage (CCS) technologies, cleaner and more efficient techniques, such as oxygen-fired combustion, and chemical looping combustion, have been implemented in CFB boilers. In oxygen-fired CFB boilers, the fuel is burned with a mixture of pure oxygen and recycled flue gas [28]. The higher level of radiating gases in oxygen fired combustion limits the use of spectral radiation models, which are developed for conventional air-fired combustion systems [3, 6, 4].

The predictions of the present method for the case study of the back pass channel were compared with those of the gray gas model. The computational costs of two different RTE solvers, i.e., the discrete ordinate method (DO) and the P1 approximation method, were compared when different spectral models were used. Finally, the effect of different operational parameters on the heat transfer within the back pass channel was considered.

#### **Banded Approach Theory**

P1 and DO are two widely used RTE solvers in engineering CFD calculations for combustion systems. P1 performs best when it is used in optically thick media with  $\beta L \gg 1$ , whereas DO is applicable to all optical thicknesses. However, both methods are well suited for the systems in this study, namely large-scale combustion systems.

P1 is the simplified form of a more general model of the PN approximation method (or spherical harmonics method) in which the radiative intensity is expanded into an orthogonal series of spherical harmonics [2] as follows:

$$I_{\lambda}(r,\hat{s}) = \sum_{l=0}^{\infty} \sum_{m=-1}^{l} I_{\lambda,l}^{m}(r) Y_{\lambda,l}^{m}(\hat{s})$$
(1)

where  $I_{\lambda,l}^m(r)$  corresponds to the variation in intensity with position, and  $Y_{\lambda,l}^m(\hat{s})$  are the spherical harmonics that satisfy Laplace's equation in spherical coordinates. The details of the theory of the model are well documented in radiation heat transfer textbooks [2]. By using P1, the transfer equation for spectral incident radiation  $(G_{\lambda})$  is

$$\nabla (\Gamma_{\lambda} \nabla G_{\lambda}) - \kappa_{\lambda} G_{\lambda} + 4\kappa_{\lambda} n^2 \sigma T^4 = S_{G\lambda}$$
<sup>(2)</sup>

where  $\Gamma_{\lambda}$  is defined by

$$\Gamma_{\lambda} = \frac{1}{3\beta_{\lambda} - C\sigma_{S\lambda}} \tag{3}$$

in which  $\kappa_{\lambda}, \sigma_{S\lambda}, \beta_{\lambda}$ , and *C* represent the spectral absorption coefficient, spectral scattering coefficient, spectral extinction coefficient, and the linear scattering phase function coefficient, respectively.  $S_{G\lambda}$  represents an additional source of incident radiation, if there is any.

For non-gray gas modeling by the proposed banded approach, the incident radiation in each band is obtained by solving this differential equation using the gray band absorption coefficient obtained by narrow band calculations. Then, the spectral radiative heat flux is calculated as follows:

$$q_{\lambda} = -\Gamma_{\lambda} \nabla G_{\lambda} \tag{4}$$

and its divergence or radiative source term in each band is

$$RST_{\lambda} = -\nabla q_{r,\lambda} = \kappa_{\lambda} \left( G_{\lambda} - n^2 E_{b\lambda} \right)$$
<sup>(5)</sup>

in which  $G_{b\lambda}$  is the spectral black body emission, which for each band is

$$E_{b\lambda} = 4 \left( f(n\lambda_2 T) - f(n\lambda_1 T) \right) \sigma T^4$$
(6)

where  $f(n\lambda T)$  is the fraction of the blackbody emissive power contained between 0 and  $n\lambda T$ , and  $\lambda_1$  and  $\lambda_2$  are the wavelength limits of the bands. The wall boundary conditions should be implemented on a banded base. For instance, the radiative heat flux leaving a non-gray wall in a specific band is

$$q_{out,\Delta\lambda} = \left(1 - \varepsilon_{w,\Delta\lambda}\right) G_{\Delta\lambda} + \varepsilon_{w,\Delta\lambda} \left(f(n\lambda_2 T) - f(n\lambda_1 T)\right) n^2 \sigma T_w^4 \tag{7}$$

and the surface radiation incident on the selected spectral interval  $\Delta \lambda$  is

$$G_{\Delta\lambda} = \Delta\lambda \int_{s,n>0} I_{\lambda} \,\hat{s}.\hat{n} \,d\lambda \,. \tag{8}$$

The other widely used RTE solver is DO, which solves the RTE for a finite number of discrete solid angles, each associated with a vector direction fixed in a coordinate system. In the DO method, the angular variation in the radiation intensity is represented discretely, and the angular integration is replaced by a quadrature summed over each discrete ordinate [29]. The discrete ordinate form of the RTE for the spectral radiation intensity in an absorbing, emitting, but not scattering media is written as

$$\xi^{m} \frac{dI_{\lambda}^{m}}{dx} + \eta^{m} \frac{dI_{\lambda}^{m}}{dy} + \mu^{m} \frac{dI_{\lambda}^{m}}{dz} + \kappa_{\lambda} I_{\lambda}^{m} = \kappa_{\lambda} I_{b\lambda}$$
<sup>(9)</sup>

where  $\xi^m$ ,  $\eta^m$ , and  $\mu^m$  are the direction cosines associated with the ordinate m,  $I_{\lambda}$  is the radiation intensity in each band,  $\kappa_{\lambda}$  is the gray band absorption coefficient, and  $I_{b\lambda}$  is the

blackbody radiation intensity associated with the band, which is defined as  $(f(n\lambda_2 T) - f(n\lambda_1 T))\sigma T^4 / \pi$ .

Eq. (7) can be solved by the conventional finite volume method for each ordinate and each band. The boundary conditions at the walls are

$$I_{\lambda,w}^{m} = \varepsilon_{\lambda,w} I_{b\lambda,w} + \frac{1 - \varepsilon_{\lambda,w}}{\pi} \int_{\hat{n}.\Omega' < 0} \left| \hat{n}.\Omega' \right| I_{\lambda,w}(\Omega') d\Omega' \qquad for \ \hat{n}.\Omega' > 0$$
<sup>(10)</sup>

After the radiative intensity field has been obtained, the radiation incident and radiative heat flux are

$$G_{\lambda} = \sum_{m} w_{m} I_{\lambda}^{m} \tag{11}$$

$$q_{\lambda} = \sum_{m} \mu^{m} I_{\lambda}^{m} w^{m}$$
<sup>(12)</sup>

where  $w_m$  represents the weight of the ordinates. The radiative source term can be obtained from Eq. (5) or as the negative divergence of the radiative heat flux.

For both RTE solvers, the total radiative heat flux and radiative source term will be then obtained by performing a summation over all bands.

## **Narrow Band Calculations**

The SNB calculation is well known as one of the most accurate models for estimating the spectral radiation heat transfer in molecular gases [2, 14]. In this method, the entire radiative heat transfer spectrum is divided into narrow wavenumber intervals. In each narrow band, the absorption coefficient varies widely. However, by assuming a certain statistical distribution for the absorption lines within the narrow bands, the SNB models calculate the transmissivity of a gas layer with a certain thickness. The model parameters were obtained in [30, 31] by using the most up-to-date line-by-line databases. By using the Malkmus model [32] with the Lorentz line shapes [33], the transmissivity averaged over a wide spectral interval of a homogeneous and isothermal slab of a gas is [31]

$$\overline{\tau}^{\Delta\eta} = \exp\left[-2\frac{\overline{\gamma}}{\overline{\delta}}\left(\sqrt{1 + \frac{\chi P_t l \,\overline{k} \,\overline{\delta}}{\overline{\gamma}}} - 1\right)\right] \tag{13}$$

where *l* is the path length (cm),  $P_l$  is the total pressure (bar),  $\chi$  is the molar fraction,  $\overline{k}$  (cm<sup>-1</sup>) is the mean line intensity to line spacing ratio,  $\overline{\delta}$  (cm<sup>-1</sup>) is the average line Lorentz halfwidth, and  $\overline{\gamma}$  (cm<sup>-1</sup>) is the mean line spacing.

The model parameters  $\overline{k}$  and  $\overline{\delta}$  for each single gas have been obtained by line-by-line calculation for four different combustion gases, i.e., H<sub>2</sub>O, CO<sub>2</sub>., CO, and CH<sub>4</sub> [31]. The last parameter of the model is the average line Lorentz half-width ( $\overline{\delta}$ ), which is calculated for H<sub>2</sub>O and CO<sub>2</sub> by [31], namely

$$\overline{\gamma}_{H_2O} = \frac{p}{p_s} \left\{ 0.462 \frac{T_s}{T} \chi_{H_2O} + \left(\frac{T_s}{T}\right)^{0.5} \times \left[ 0.0792(1 - \chi_{CO_2} - \chi_{O_2}) + 0.106 \chi_{CO_2} + 0.036 \chi_{O_2} \right] \right\}$$
(14)

$$\overline{\gamma}_{CO_2} = \frac{p}{p_s} \left(\frac{T_s}{T}\right)^{0.7} \left[ 0.07 \chi_{CO_2} + 0.058(1 - \chi_{CO_2} - \chi_{H_2O}) + 0.1 \chi_{H_2O} \right]$$
(15)

In these two equations,  $p_s = 1 atm$  and  $T_s = 296K$ .

The parameters of the SNB model were obtained with a constant 25 cm<sup>-1</sup> spectral width using the LBL calculations, including all the lines in the HITRAN database [34]. Rivière et al. [35] showed that this width is sufficiently narrow to assume a constant Planck function inside each band for the temperature range 300–2500 K. After obtaining the transmissivity of the individual gas species by Eq. 13, one can calculate the transmissivity of the gas mixture by multiplying the transmissivities of all gas species.

In this study, the SNB model was used to calculate the transmissivity of a layer of the homogeneous gas mixture with a specific path length. The mean absorption coefficient of the gas mixture in each narrow band can then be obtained by applying Beer's law as follows:

$$k_{\lambda} = -\ln(\overline{\tau}_{mix}) / \left( \left( \chi_{CO2} + \chi_{H2O} \right) P_t l \right)$$
<sup>(16)</sup>

Although the approach of using a mean absorption coefficient for a narrow band is not exact, it may be justified in engineering calculations because it significantly reduces computational time. Figure 1 shows two sample profiles of the spectral absorption coefficient obtained from the SNB model. The gas compositions in the cases illustrated in this figure correspond to the typical air-fired and oxygen-fired combustion.

#### **Correlations for Band Absorption Coefficients**

In this study, the simplified SNB model was used, where the mean absorption coefficient of a homogeneous column of a gas mixture is calculated by Eq. 16 to obtain the gray band absorption coefficient of the considerably wider bands used in the present banded approach. In each wide band, the mean absorption coefficient was obtained using the narrow band data of the absorption coefficients weighted by the blackbody intensity as follows:

$$\bar{\kappa}\big|_{\lambda_1-\lambda_2} = \frac{\int_{\lambda_1}^{\lambda_2} I_{b,\lambda} k_{\lambda} d\lambda}{\int_{\lambda_1}^{\lambda_2} I_{b,\lambda} d\lambda}$$
(17)

To divide the thermal radiation spectrum into a limited number of bands in which the RTE should be solved, the band dividing scheme by Maximov in [25] was adopted. By testing several dividing schemes on certain benchmarks, he reported 10 wavelength intervals (shown in Table 1) as the optimal dividing scheme for non-gray gas modeling of air and oxygen-fired combustors. It is worth noting that thermal radiation generally occurs in 0.1–100  $\mu$ m. However, by detailed spectral analysis corresponding to a wide range of thermal conditions in combustion systems, Maximov [25] demonstrated that for high-temperature CO<sub>2</sub>-H<sub>2</sub>O mixtures under variant combustion conditions, the most significant contribution of CO<sub>2</sub> and H<sub>2</sub>O absorption and emission occurs within the identified bands, whereas the contribution of other spectral parts is small and can be assumed negligible. In fact, those regions (including  $\lambda < 1.338 \ \mu$ m and  $\lambda > 66.67 \ \mu$ m) represent the windows between the active bands.

Table 1: Recommended band limits for CFD calculations in the non-gray banded approach.

Band No.	1	2	3	4	5	6	7	8	9	10
Start (µm)	1.338	1.77	2.454	2.632	4.167	5.263	6.154	8.889	12.90	16.67
End (µm)	1.465	2.105	2.632	2.878	4.706	5.970	7.843	12.90	16.67	66.67







(b)

Figure 1. Spectral absorption coefficient of a  $H_2O$ - $CO_2$  mixture at two different temperatures calculated by the SNB method. (a) represents air-fired combustion with 20%  $H_2O$  and 10%  $CO_2$ , and (b) represents oxy-fired combustion with 10%  $H_2O$  and 85%  $CO_2$  (molar basis).

To provide simple correlations for the gray band absorption coefficients that should cover a wide range of thermodynamic states in practical combustion systems, the SNB model was implemented to provide databases of gray band absorption coefficient of the bands introduced in Table 1. Databases were obtained for molar fraction ratios ( $M_r = \chi_{H_2O}/\chi_{CO_2}$ ), of 1/8 (corresponding to dry flue gas recycling), 1/4, 1/2, 1 (corresponding to wet flue gas recycling), and 2, where in all cases it is assumed that  $p_{CO2} + p_{H2O} = 1 a tm$ . It should be noted that despite this assumption, by considering the partial gas pressure in the final correlations, the databases are applicable to other situation where there is gases such as nitrogen and oxygen which are neutral to radiation heat transfer. For each molar fraction ratio, the band absorption coefficients were determined for temperatures between 500 and 2400 K with a step of 100 K and for 200 path lengths between 10 cm and 15 m. Therefore, each database corresponding to a certain gas composition contains 4400 points for each band, covering the most practical combustion conditions.

The following form of correlation was implemented to approximate the band absorption coefficient databases:

$$\bar{\kappa} = a_1 + a_2 \ln(T) + a_3 \ln(PL) + a_4 \ln(T)^2 + a_5 \ln(PL)^2 + a_6 \ln(T) \ln(PL)$$
<sup>(18)</sup>

where  $PL = (\chi_{CO2} + \chi_{H2O})P_tL$  in which L is the spectrally averaged mean beam length [2]. Maximov [25] used the same form of correlation for the band absorption coefficients of a H<sub>2</sub>O-CO<sub>2</sub> mixture for oxygen-fired combustion conditions. To include the effect of the molar fraction ratio, Maximov used a two-step fitting procedure. He first obtained the coefficients of his correlation for each molar fraction ratio, and then he expressed the dependency of the coefficients on the molar fraction ratio of the gas mixture by a polynomial function. He obtained three sets of coefficients for three different ranges of pressure path length products (PL). In each PL range, he reported only one set of coefficients for the entire range of molar fraction ratios occurred in oxygen-fired combustion conditions. However, as the function of the correlation is strongly nonlinear, using the previously mentioned two-step fitting to incorporate the effect of the molar fraction ratio induces some uncertainty, particularly for the thermal conditions that do not correspond to database points. Thus, in the present study, the coefficients in (18) were separately determined for each molar fraction ratio of interest. For molar fraction ratios that do not correspond to the tabulated coefficients, linear interpolation/extrapolation is recommended between the values of the band absorption coefficients obtained by correlations for the tabulated molar fraction ratios. In addition to accuracy, another advantage is the support of both air- and oxygen-fired conditions using the same form of correlation and coefficients.

By using the obtained narrow-band-based databases of the band absorption coefficients, the Matlab LSQCURVEFIT function was employed for curve fitting. This function is based on the nonlinear least squares method, whereby the best curve parameters are obtained for which the square of the error between the values from the fitting equation and the target vector is minimized. The coefficients of the correlations obtained for each molar fraction ratio are given in Appendix. Moreover, a user defined function (UDF) has been provided as a supplementary material of this article to ease implementation of the proposed model in nongray gas modeling with Ansys-Fluent CFD solver.

## Validation

## **Study of One-Dimensional Slab Problems**

Radiation heat transfer in participating media bounded between two infinite parallel plates, i.e., a slab problem, has been widely used to validate new RTE solvers and spectral radiation models [8, 14, 18, 3]. To validate the present approach and to study its performance including its accuracy and computational cost in variant thermodynamic conditions, we also implemented it in several slab problems. RTE is solved by the DO method using S8 solid angle discretization [2]. Following [8, 3] the line-by-line spectral absorption coefficient profile obtained from HITEMP2010 [34] was used as the reference solution to evaluate other spectral methods. The LBL gas absorption spectrum was obtained for a range of 150–15000 cm<sup>-1</sup> (0.66–66.67  $\mu$ m) with a resolution of 0.02 cm<sup>-1</sup>. This covers the entire thermal radiation spectrum of combustion systems in the range of interest with very fine resolution and therefore provides the exact benchmark solution.

Case No.	$\epsilon_{wall}$	Twall (K)	L (m)	Mr	T (K)	$\chi_{H_2O}$ (-)	<i>χ</i> <sub>CO2</sub> (-)
1	1 (Black)	300	1	2	1000	0.2	0.1
2	Non-gray; Fig. (3)	500	1	Inf.	1000	0.5	0.0
3	Non-gray; Fig. (3)	500	1	0	1000	0	0.1
4	Non-gray; Fig. (3)	500	0.1	4/3	Fig. 6	Fig. 6	Fig. 6

Table 2: Thermal conditions for 1D benchmarks.



Figure 2. Radiative heat flux (top) and radiative heat source of different models for case 1.

In addition to the LBL solution, which is assumed to be exact, the predictions of the present 10-band model were compared with those by four other models, namely Bordbar's WSGG [8], Smith's WSGG [17], Bordbar's 31-band model [3], and Maximov's 10-band model [25]. These four cases represent various thermal conditions. Case 1 involves a mixture of both gases in homogeneous condition bounded between two black walls at T = 300 K, whereas in cases 2 and 3, only one of the gases is in homogeneous condition bounded between two non-gray walls. The gas compositions in the first three cases correspond to the Mr values in which the parameters of the models were obtained and tabulated, whereas in case 4, completely inhomogeneous temperature and gas composition profiles were considered, resulting in a molar fraction ratio that is not tabulated in any of the considered models. The length in case 4 and hence the optical thickness are considered significantly smaller than in the other cases so that the performance of the models in optically thin conditions may be addressed.

Figure 2 shows the radiative heat flux and radiative heat source along the line between the infinite parallel plates. All models exhibit a quite satisfactory level of accuracy. Bordbar's WSGG model yields the most accurate results in the entire length, whereas Bordbar's 31-band model [3] and Smith's WSGG [17] are least accurate especially in close to wall regions. The present model and Maximov's model [25] yield quite similar results, with slightly better accuracy for the present model. It should be noted that the wall temperature for case 1 is out of the range of the present model, and this may partially account for the model's inaccuracy in this case.

To study the performance of different approaches in supporting spectrally dependent wall emittance, a symmetric quadratic profile, described by Eq. 19, has been considered for cases 2–4.

$$\varepsilon_{wall} = \begin{cases} -0.0711 \left(\frac{\eta}{1000}\right)^2 + 0.533 \left(\frac{\eta}{1000}\right) & \eta \le 7500 \ cm^{-1} \\ 0 & \eta > 7500 \ cm^{-1} \end{cases}$$
(19)

It is worth noting that even though the LBL solution may have a variant wall emittance profile with high resolution, the other methods should use averaged values of spectral emittance, representing the high-resolution profile. The global models, such as WSGG, cannot support non-gray walls because they are based on wavenumber reordering and therefore can support only an averaged value for the wall emittance over the entire spectrum, i.e., gray walls. This averaged value for the present non-gray profile is 0.3363. By contrast, the banded approach can more accurately consider the variation in wall emittance with wavenumber. The

averaged values of spectral wall emittance are used over the bands. The averaged values of wall emittance in different bands for different models are shown in Figure 3.



Figure 3. Spectral wall emittance for cases 2–4 with non-gray walls.

Case 2 involves homogeneous water vapor bounded between two non-gray walls; thus, the molar fraction ratio is infinite. This is not supported by Bordbar's WSGG and Maximov's models. The comparison of the predictions by the other three models with LBL data is shown in Figure 4. For this case, Bordbar's 31-band model shows the best agreement with the LBL data for the radiative heat flux; however, its prediction for the radiative source term is not as accurate, particularly for regions close to walls. The present model exhibits the same level of accuracy along the entire length. It is better than Smith's WSGG model both for the radiative heat flux and the radiative source term. The predictions of the present model for the radiative source term are better than those of Bordbar's 31-band model, whereas its computational time is significantly shorter.



*Figure 4. Radiative heat flux (top) and radiative heat source of different models for case 2.* 



*Figure 5. Radiative heat flux (top) and radiative heat source of different models for case 3.* 

Case 3 involves only CO2 in homogeneous conditions bounded between two non-gray walls. Figure 5 shows the predictions of different models for this case. The present method is slightly less accurate than Bordbar's 31-band model but significantly more accurate than Maximov's 10-band model and the two WSGG models. The computational time of the present model, as reported in Table 3, is almost 41.5 times less than that of Bordbar's 31-band model and 8.6 times less than that of Maximov's 10-band model.

Case 4 represents an inhomogeneous medium bounded between two non-gray walls. The temperature and gas molar fractions follow symmetric quadratic profiles having the minimum values at the two walls and the maxima in the middle, as shown in Figure 6.



Figure 6. Inhomogeneous profiles of temperature and gas composition of case 4.



Figure 7. Radiative heat flux (top) and radiative heat source of different models for case 4.

The predictions of different models for case 4 were compared with those of the LBL calculations in Figure 7. In terms of accuracy, the present approach is at the same level as Bordbar's 31-band model and significantly better than Maximov's 10-band as well as the two WSGG models.

The computational time per computational cell for models in all cases is shown in Table 3. To provide a fair comparison, all codes were written in the same programing language and using the same coding methodology; furthermore, CPU time was measured on the same computer in identical conditions. The computational cost of the present approach for all cases is almost twice as much as that of the WSGG models. However, it is almost 29 times less than that of Maximov's 10-band model and almost 160 times less than that of Bordbar's 31-band model for cases 1–3, as shown in Table 3. For case 4, under inhomogeneous conditions and when Mr does not correspond to any tabulated Mr point of the models, the computational time of all models except Bordbar's 31-band model increases, owing to the superposition techniques used in that model for calculating the band absorption coefficient of the mixture by using the band absorption coefficients of individual gases weighted by their mole fraction. Thus, the computational time of that model was nearly constant for all cases. However, in case 4, the present model is 8.66 times as fast as Maximov's method, 2.3 times as slow as Bordbar's WSGG, and 3.95 times as slow as Smith's model.

	Number	Present 10-	Bordbar's	Maximov's	Bordbar's	Smith's
	of cells	band model	31-band [3]	10-band [25]	WSGG [8]	WSGG [17]
Case 1	101	0.379	62.863	10.930	0.139	0.062
Case 2	101	0.395	63.908	-	-	0.125
Case 3	101	0.401	64.194	11.247	0.177	0.217
Case 4	21	1.291	63.808	11.179	0.562	0.327

Table 3. Computational time per computational cell (ms) of different models

To provide a better quantitative view of the accuracy of the models, the mean square error of the calculated radiative heat flux and radiative source term is reported in Tables 4 and 5, respectively. Overall, the accuracy and computational time of the WSGG models are better for case 1, where the walls are black. However, these models cannot support non-gray walls and are limited to using a spectrally averaged value for wall emittance. Hence, their accuracy in cases 2–4 with non-gray walls is poor. As the banded approach is based on the averaging of

the absorption coefficients within the actual spectral location, these models can more accurately support the spectrally dependent radiative properties of the walls. This is in contrast to global models, which are based on wavenumber reordering and use pre-integrated spectral radiative properties in solving the RTE over the reordered wavenumber. This is clearly seen in the results for cases 2–4.

In case 4, where there is an inhomogeneous condition in optically thin conditions, all models except for the present model are less accurate than in the other cases under the homogeneous condition. For Bordbar's WSGG model and Maximov's 10-band model, this is primarily due to the inaccuracy induced by the two-step fitting. In these two models, after the model parameters for molar fraction points have been obtained, polynomial functions are fitted over the model parameters, providing a single set of coefficients for the entire range of the molar fraction ratio. For Maximov's model, this process was carried out for three different ranges of optical thickness. Although this reduces the size of the model parameters, it also reduces accuracy under conditions that do not correspond to tabulated molar fraction ratios.

	Present 10-	Bordbar's	Maximov's	Bordbar's	Smith's
	band model	31-band [3]	10-bands [25]	WSGG [8]	WSGG [17]
Case 1	13.6	14.38	18.47	1.78	7.27
Case 2	31.59	14.13	-	-	64.6
Case 3	19.99	10.62	77.24	39.89	49.61
Case 4	12.48	11.14	13.31	18.33	23.24

Table 4. Mean square error (%) of radiative heat flux

Table 5. Mean square error (%) of radiative heat source calculated by different models

	Present 10-	Bordbar's	Maximov's	Bordbar's	Smith's
	band model	31-band [3]	10-band [25]	WSGG [8]	WSGG [17]
Case 1	15.7	18.40	19.22	4.13	9.41
Case 2	28.3	16.13	-	-	61.1
Case 3	22.20	16.13	79.98	41.78	52.95
Case 4	16.63	28.33	23.16	79.00	56.83

#### **Three-Dimensional Benchmarks**

To validate the model, two air and oxy-fired combustion benchmarks were used. Specifically, a rectangular enclosure of  $2 \text{ m} \times 2 \text{ m} \times 4 \text{ m}$  with black surrounding walls at 300 K was used. The temperature distribution is symmetrical about the geometric centerline and given by

$$T = (T_c - T_e)f(r_c / R) + T_e$$
<sup>(19)</sup>

where  $T_c$  is the gas temperature along the geometric centerline and  $T_e$  is the temperature at the geometric exit at z = 4 m.  $f(r_c/R)$  is the variation in the gas temperature inside a circular cross section around the centerline and is defined by

$$f(r_c / R) = 1 - 3(r_c / R)^2 + 2(r_c / R)^3$$
(20)

where R = 1. The temperature along the centerline  $(T_c)$  increases linearly from 400K at z = 0to a maximum value of 1800K at z = 0.375m, and then linearly decreases to  $T_e = 800K$  at the exit section z = 4m. The mole fractions of CO<sub>2</sub>, H<sub>2</sub>O, and N<sub>2</sub> in the air-fired benchmark are 0.1, 0.2, and 0.7, respectively, whereas the mixture in the oxygen-fired benchmark consists of 85% CO<sub>2</sub>, 10% H<sub>2</sub>O, and 5% N<sub>2</sub>. There are a number of solutions in the literature for these benchmarks. Liu [26] and Porter et al. [27] used the ray tracing (RT) method together with the SNB model. Clements et al. [36] evaluated the performance of FSCKM with different numbers of quadrature points for the oxy-fired benchmark.

The benchmark problem was solved by a CFD solver, i.e., Ansys-Fluent R16.0, in a computational grid of  $17 \times 17 \times 24$  with uniform grid divisions in the *x* and *y* directions and nonuniform grid divisions in the *z*-direction with a finer grid around the peak temperature at z = 0.375m. This grid was chosen to be the same as in [26] and [27] so that the results may be compatible with the benchmark solutions. The RTE was solved by the DO method with an angular discretization of  $N_{\theta} = N_{\phi} = 4$ . Using finer angular discretization does not significantly alter the results [36].

The results of the present approach were compared with those by the non-gray implementation of WSGG, the FSCK model, and SNB-RT [26]. Recently, two sets of coefficients were reported for WSGG models in air [5] and oxygen-fired [8] conditions. They were obtained by line-by-line calculations using the HITEMP 2010 spectral database [34]. These two sets of WSGG coefficients were used for the evaluation of the present box model. Kez et al. [37]

recently compared different radiative property models for oxygen-fired combustors with a dry flue gas recycle and concluded that the WSGG coefficients reported by Bordbar et al. [8] represent the best available non-gray gas model for practical use.

Figure 8 shows the results of the present box model for the radiative heat flux on the line (2,1,z) on the side of the air-fired benchmark setup. In this figure, for all models except for the narrow band model, the DO method with an angular discretization of  $N_{\theta} = N_{\phi} = 4$  was used as the RTE solver. For the narrow band model, the ray tracing method was used. The results of the present box model are in the range of the reported results for non-gray gas models and are closest to the reported results of the narrow band model (RT+SNB). The results of the gray gas Smith's WSGG model, which is used in Fluent, are the least accurate because the total emissivity of the mixture is calculated by assuming the mean beam length. The results of FSCK were obtained by using the recently published look-up table [18] with seven quadrature points.



Figure 8. Radiative heat flux on the line (2,1,z) of the air-fired benchmark calculated by the present box model compared with the results of some other radiative property models.

Figure 9 shows the results of the present box model for the radiative source term on the center line (0,0,z) of the oxy-fired benchmark setup. The P1 method was used as the RTE solver. The results of the present box model are in good agreement with those of other non-gray gas models.

It should be noted that part of the deviation in the results of all models is because different RTE solvers were used in the predictions of the simpler models and the benchmark solution. The RTE solver in the benchmark solution was the ray tracing method, which is expected to yield the most accurate solution at rather high computational cost.



Figure 9. Radiative source term on the center line (0,0,z) of the oxy-fired benchmark calculated by the present box model compared with the results of some other radiative property models.

#### **Application to a Combustion System**

CFB technology has been widely used for combustion of solid fuel. It has several advantages, such as fuel flexibility, high combustion intensity, and low emissions [38]. In most gas particle combustion systems, particle radiation is significant and should be carefully modeled [39, 40, 41, 42]. Passing the cyclone, which is located immediately after the furnace, most of the particles are separated from the flue gas flow and return back to the furnace. The solid mass fraction is significantly smaller than the gas mass fraction in the hot flue gases exiting from the cyclone and flowing to the back pass channel. The particle volume fraction is on the order of 10<sup>-6</sup>, and the mean particle size allows the use of geometric optics for calculating the particle absorption and scattering coefficient as in [39]. Following [39], the extinction coefficient of the particle phase for this large-scale back pass channel has been estimated to be a small

percentage of that of the gas phase. Hence, in the back pass channel of the selected CFB boiler, the contribution of the particles in the radiative heat transfer is quite small and was assumed negligible compared to that of gas thermal radiation. This assumption was validated by operational data of the back pass channel. In fact, in the back pass channel, the gas dominates the thermal radiation, and therefore the radiation modeling can be performed by considering the effect of the gas [1]. This makes the effect of non-gray gases more evident. Ates et al. [43] showed that the gray assumption for particles in fluidized systems leads to accurate radiative heat flux predictions, and therefore for the regions where the particle contribution in the overall thermal radiation is significant, for instance in CFB furnaces, one can add the gray particle absorption coefficient to the gray band gas absorption coefficient in each band. The procedure is the same as in calculation of the radiative properties of gas particle mixtures in gray models [39] or in the WSGG model [44].

The present box model was used to analyze the radiative heat transfer in the back pass channel of a CFB boiler in air and oxygen-fired combustion modes. The geometry and model for this analysis are shown in Figure 10. A diagram of the CFB appears in [1].



Figure 10. Geometry and model of back pass channel of a CFB boiler.

The conditions of gas flow in the inlet sections correspond to an air-fired combustion scenario  $(x_{H2O} = 9.7\%, x_{CO2} = 14.3\%, x_{N2} = 71.9\%)$  and an oxygen-fired combustion scenario  $(x_{H2O} = 21\%, x_{CO2} = 70\%, x_{N2} = 1.8\%)$ . The remainder of the gas mixtures consists of Ar, SO<sub>2</sub>, and O<sub>2</sub>, which are assumed to be neutral to radiation. The standard k-epsilon model was used for turbulent modeling, and the present box model, together with two RTE solvers, i.e., DO and P1, were used for non-gray gas modeling. The results are compared with those by the Fluent gray gas model (gray Smith's WSGG). It should be noted that to implement WSGG for gray

modeling, the mean beam length should be estimated, which, in common practice, is obtained based on the domain size by the formula  $3.6 \times V/A$ , where V and A represent the volume of the participating media and its surronding area, respectively.

To ensure that the model is mesh-independent, the results of two different grid structures were compared for the radiative heat flux on line 1, shown in Figure 10, and the temperature along the geometric axis. The study corresponds to case 4 in Table 6, in which the temperature of the inlet flow is 950°C and is evenly distributed across all the inlet sections. The combustion mode is air-fired, and all walls are assumed to be black at a constant temperature of 480°C. The number of cells in the finer mesh structure (1255900) is nearly eight times as large as in the coarser grid (154800). The normalized temperature is defined as  $T/T_{max}$ , and the normalized radiative heat flux is also defined as  $q_r/q_{r,max}$ , where  $T_{max}$  and  $q_{r,max}$  represent respectively the maximum temperature along the axis line and the maximum radiative heat flux along line 1 in two different grids. The results shown in Figure 11 were obtained by using P1 as the RTE solver together with the present box model. The radiative heat powers of the unit obtained by the two different mesh structures differ by only 0.4%, and the maximum values of temperature and radiative heat flux in the two cases differ only by 0.5% and 0.33%, respectively. This, together with Figure 11, demonstrates the mesh independency of the analysis and, owing to the considerably higher computational cost of the finer structure, justifies the use of the coarser grid structure.



Figure 11: Mesh independency analysis. Profile of normalized temperature along the axis line of the geometry and normalized radiative heat flux along line 1 shown in Figure 10 obtained by P1 together with the present box model.

Bordbar et al. [1] used the zone method and various WSGG models to analyze the radiative heat transfer in a back pass channel of a CFB boiler. The dimensions of the model in that study were slightly different from those in the present study, but the operational and wall boundary conditions are the same as those of case 4 in Table 6. Although the dimensions in the two studies are slightly different, the results of the two models should still be quantitatively comparable. Figure 12 shows the normalized radiative heat flux along line 1 shown in Figure 10. The non-gray gas results of the present box model are in quantitatively good agreement with the previously reported results of non-gray gas modeling by the zone method [1] implementing the WSGG model with the coefficients reported by Smith et al. [17] for air-fired combustion. Because the size of the zone used in the previous study [1] was quite large (45 cm), the radiative heat flux had low resolution at the beginning and the end of the line. This is the main cause of the differences between the results by the zone method and those by the present non-gray box model.



Figure 12: Normalized radiative heat flux along line 1 shown in Figure 10. The results of the present non-gray box model implemented in DO have been compared with the previously reported results of the non-gray zone method and also gray WSGG.

To study the effect of the boiler load (inlet temperature), the wall boundary condition (membrane wall or refractory lines), and the number of inlets on the heat transfer within the unit, the cases in Table 6 are considered.

Table 6. Effect of different operational conditions on the heat transfer in the back pass channel.

	Gas		Gas temperature		Wall surface		Gas inlet source		
	comp	osition							
Case	air	оху	low	med.	High	Metal	refrac.	all (4)	firs (1)
No.									
1	air				950	(480°C)	calc.	4	
2	air			850		(480°C)	calc.	4	
3	air		750			(480°C)	calc.	4	
4	air				950	480°C	-	4	
5	air				950	(480°C)	calc.		1
6		oxy			950	(480°C)	calc.	4	
7		oxy		850		(480°C)	calc.	4	
8		oxy	750			(480°C)	calc.	4	
9		oxy			950	480°C	-	4	
10		oxy			950	(480°C)	calc.		1

For the cases in which the walls of the geometry are refractory, the wall boundary condition is derived from a problem of 1D conduction in the refractory layer. In these cases, the temperature of the water side is fixed at 480°C, and the thickness of the refractory layer is 37 mm, with a conductivity of 0.94 W/(mK).

The radiative, convective, and total heating power of the entire heating walls of the back pass channel was obtained by CFD calculations. Two RTE solvers, P1 and DO, were used. The solid angle discretization in the DO method is  $N_{\theta} = N_{\phi} = 4$ . Both solvers were implemented in the gray WSGG [17] model and the present non-gray gas box model.

It should be noted that, as previously mentioned, P1 should be used for optically thick media ( $\beta L >> 1$ ). For non-gray gas modeling, where the RTE should be solved several times for different bands/gray gases, it is not straightforward to check a single value of  $\beta L$ , as it has

several different values for different bands/gray gases. For the case of back pass channel, the average values of gray gas band absorption coefficients over the computational domain varies considerably. As the dimensions of the system  $(5.4 \ m \times 7.2 \ m \times 27.6 \ m)$  are large, most  $\beta$ L values can be safely significantly larger than unity, and thus P1 is quite accurate. However, some values may happen to be less than unity. Hence, one can conclude that DO is preferable for non-gray gas modeling, as it is valid across the range of optical thicknesses; however, it is substantially more expensive to use.

Figure 13 shows the effect of inlet temperature on the radiative heat power of the back pass channel. P1 was used as the RTE solver, and both the gray WSGG [17] and the present nongray box model were implemented. In both combustion modes, the radiative heating power of the unit increases with the inlet temperature, as expected. The gray gas model overestimates the radiative heat power because it considers a uniform constant effective absorption coefficient for the entire radiative heat transfer wavelength spectrum. The other uncertainty that causes error in the gray implementation of WSGG is in the estimation of the mean beam length. As seen in Figure 13, the results of the box model demonstrate that the oxygen-fired combustion mode produces more power, which is physically expected owing to the higher emission of the CO<sub>2</sub>–H<sub>2</sub>O mixture. However, the results of gray gas modeling with WSGG do not exhibit such behavior because the spectral variation in the absorption coefficient is ignored and the estimation of the mean beam length is inaccurate.



*Figure 13: Changes in radiative heating power of the back pass channel with the boiler load (inlet temperature) for air and oxygen-fired combustion cases.* 



Figure 14. Effect of wall type on the radiative (RHP), convective (CHP), and total heating power (THP) of the unit in air-fired mode.

To study the effect of the wall material on the heating power of the unit, the results of the implementation of the present non-gray box model for cases 1 and 4 were compared, as shown in Figure 14. These two cases are based on the air-fired combustion mode and are completely identical except for the material of the walls, i.e., membrane metal wall or refractory lines. The temperature of the membrane wall is equal to the outside temperature of the refractory lines. Heating power is considerably higher in case 4 with membrane metal walls, owing to the higher temperature on the inside edge of the refractory lines, which causes a lower temperature difference with the flue gas flow temperature and thus less heat flux. The same trend as shown in Figure 15 is also observed in oxygen-fired mode, i.e., in the comparison between cases 6 and 9.



Figure 15. Effect of wall type on the radiative (RHP), convective (CHP) and total heating power (THP) of the unit in oxy-fired mode.



Figure 16. Effect of number of inlets on the radiative (RHP), convective (CHP) and total heating power (THP) of the unit in air-fired mode.

Figure 16 shows the change in heating power when the entire mass flow comes from only the first inlet in comparison with the case in which the inlet flow comes evenly from all four inlets. Although the cases in which the entire mass flow comes from the first inlet section, i.e., cases 5 and 10, are not practically feasible, owing to the large values of the velocity required, particularly in the first half of the channel, they have been included in this analysis to study the

effect of changes in the flow pattern on the ratio between the radiation and convection heat transfer, that is, large changes in the convection may affect the radiation heat flux. The results of the oxygen-fired combustion cases (cases 6 and 10) are shown in Figure 16 for the present non-gray gas box model. When the flow comes from all four inlets, the convective heat flux is less than when the flow comes only from the first inlet. This is due to the higher velocity in the first part of the channel in the latter case. However, this flux makes the average temperature of the flue gas less than in the case with four inlets. Thus, the radiative heat flux is lower in the case with only one inlet. By considering the effects of both radiative and convective heat fluxes, the total heat flux in the case with one inlet is slightly higher than in the case with four inlets. The same behavior was also observed in the air-fired cases with different numbers of inlets, i.e., cases 1 and 5.

In most cases, such as in Figures 14, 15, and 16, there was a small difference between the predictions of P1 and DO with a solid angle discretization of  $N_{\theta} = N_{\phi} = 4$  for the overall radiative, convective, and total heating power of the system. However, the difference between their computational costs was significant. For case 1, the computational cost of the three different RTE solvers with the gray WSGG model and the present non-gray box model are compared in Figure 17. All calculations were performed on the same machine, and the required time for one radiation iteration was then obtained. To make the results of the CPU cost analysis more general and meaningful, the obtained computational time was normalized to the maximum time. As seen in Figure 17, DO with a solid angle discretization of  $N_{\theta} = N_{\phi} = 4$ has the highest computational cost, almost twice as high as that of DO with  $N_{\theta} = N_{\phi} = 2$ . The computational cost of DO with  $N_{\theta} = N_{\phi} = 2$  is also twice as high as that of P1 for both the gray and non-gray gas calculations. The difference between the computational costs of the gray and non-gray gas models is justified by the fact that in the present non-gray box model, the RTE should be separately solved in each of the ten bands. By considering that the DO ( $N_{\theta}$  =  $N_{\phi}=2$ ) is the weakest form of DO and is less accurate than DO ( $N_{\theta}=N_{\phi}=4$ ) and because the results of P1 and DO were nearly identical in all tcases, one can conclude that P1 is the optimal choice for non-gray gas modeling with the present box model.



Figure 17. Normalized computational time of different RTE solvers and gray and non-gray models obtained for case 1.

#### **Conclusions and Remarks**

After the solution of the spectral RTE by the P1 and DO methods using the banded approach was reviewed, a statistical narrow band model was developed and used to calculate the gray band absorption coefficient in 10 bands previously reported for non-gray gas modeling of air and oxygen-fired combustors. For each band and for a wide range of temperatures and molar fractions of  $H_2O$  and  $CO_2$  found in industrial combustors, a database for the gray band absorption coefficient was obtained by the SNB. A function was then fitted to the data. The correlation-based non-gray gas banded model was then implemented using DO and P1.

As the model parameters were obtained from narrow band databases for a mixture of  $CO_2$  and  $H_2O$ , there is no need for a mixing scheme as in FSCKM or SLW. Compared to the global models, the banded approach also allows modeling non-gray walls.

The present model was validated in four different slab problem representing homogeneous and inhomogeneous, one gas only or gas mixture, and black and non-gray walls. It was demonstrated that the present model is more accurate than Maximov's model [25] and requires less computational time. Compared to a similar but more complex 31-band model [3], the proposed model is significantly faster with slightly lower, or sometimes even better accuracy. All three banded approaches demonstrated their capacity to support spectrally dependent wall emittance. The results of the present model on the 1D benchmark with black walls demonstrated that its accuracy is good, close to that of WSGG models. Hence, the present

approach provides an optimized and improved version of the banded approach that can be used in the CFD modeling of large-scale combustion systems. The model was also validated on two 3D benchmarks representing typical thermal conditions of air and oxy-fired combustion.

Although the global models exhibit promising accuracy, particularly for homogeneous single gases, implementing them in heterogeneous gas mixtures requires mixing schemes [45] or premixed absorption databases, which are usually obtained by LBL or SNB calculations [36]. This implies that implementing them in practical combustion systems requires large databases [18] and complex coding.

Moreover, it is difficult to include any other gases than  $CO_2$  and  $H_2O$  in the WSGG model, whereas extending the present box model to include the effect of other active molecular gases such as  $SO_2$  is quite straightforward.

Based on the comparisons and the features of the method, it is concluded that the developed banded spectral radiation approach and the correlations can be applied in fast and accurate CFD simulations for enclosures with non-gray walls. In addition, the present model and parameters can be readily applied in CFD simulations and codes supporting banded radiation models.

After validation on several 1D and 3D benchmarks, the proposed method was used for modeling the radiative heat transfer in a large back pass channel of a CFB boiler. The model predictions were quantitatively in good agreement with the results of the non-gray zone method previously reported for nearly the same system.

The effect of the boiler load (inlet temperature), the combustion mode (air vs oxygen fired), the wall type (metal vs refractory), and the number of inlets on the heat transfer of the back pass channel was studied using the present non-gray gas banded approach and the gray WSGG model of Smith et al. [17] with the domain-based mean beam length available in the commercial CFD software package Ansys-Fluent R16.0.

It was demonstrated that the gray WSGG model in Ansys-Fluent may overestimate the radiative heat flux. No significant differences were observed between the radiative heat powers of the unit obtained by DO with  $4 \times 4$  and P1, although the computational cost of P1 was significantly lower than that of DO.

A higher inlet temperature can cause higher radiative, convective, and total heating power, as expected, and the oxygen-fired mode has a larger radiative heating power owing to the increased gas emission in this mode.

The radiative fluxes in the cases with a membrane wall at a fixed temperature were considerably larger than those of refractory lines. This was primarily due to the lower temperature difference between the walls and the flue gas flow in the case of refractory walls. When the entire mass flow enters the unit from a single inlet, the convective heating power of the unit improves owing to the larger flow velocity, whereas the radiative heat flux decreases owing to the lower temperature difference caused by the larger convective heat loss in the flue gas flow. Summing up the effects of the convection and radiation heat transfers, the total heating power of the unit is slightly greater in the cases with only one inlet section.

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Appendix I: Tables of the coefficients for the correlations of the band absorption coefficients for the air and oxygen-fired combustion scenarios.

BAND NO.	A <sub>1</sub>	$A_2$	A <sub>3</sub>	A4	A5	A <sub>6</sub>
1	1.985829	-0.169898	-0.648576	-0.007143	-0.003844	0.081536
2	1.209332	-0.234023	-0.267457	0.016826	-0.000063	0.026499
3	18.333130	-3.842048	-2.470255	0.213103	0.055931	0.260911
4	19.790020	-3.751522	-3.361840	0.182403	0.080064	0.356732
5	-1.142476	0.217618	0.120564	-0.003124	-0.002225	-0.021402
6	20.849680	-4.122157	-3.257602	0.214057	0.083781	0.339288
7	18.192440	-3.654740	-2.814294	0.216805	0.133542	0.229317
8	14.545720	-4.902579	0.895729	0.414010	0.001129	-0.145340
9	15.693150	-6.305280	3.299291	0.621025	0.048814	-0.568111
10	11.076100	-2.645757	-0.735311	0.265270	0.382563	-0.260229

Table A.1: Coefficients for the correlations of the band absorption coefficient for pureH2O at atmospheric pressure.

Table A.2: Coefficients for the correlations of the band absorption coefficient for pu	re
CO2 at atmospheric pressure.	

BAND NO.	A <sub>1</sub>	A2	<b>A</b> 3	A4	A5	A6
1	0.060643	-0.014286	-0.001099	0.000840	-0.000002	0.000142
2	0.501492	-0.098930	-0.071983	0.005336	-0.000642	0.009437
3	-0.068305	0.016185	-0.000042	-0.000738	-0.000048	-0.000023
4	9.272950	-2.656498	-0.825930	0.248210	0.046637	0.008587
5	61.627750	-24.72399	12.614520	2.734730	1.298749	-3.179420
6	0.404750	-0.125082	-0.000306	0.009740	-0.000028	0.000027
7	0.015454	-0.004939	0.000014	0.000395	0.000000	-0.000002
8	0.173689	-0.379901	0.282935	0.060332	-0.003043	-0.049357
9	21.840880	-7.039825	0.275633	0.707394	0.275312	-0.404064
10	0.998090	-0.764430	0.546698	0.105802	0.009654	-0.106379

BAND NO.	A1	A <sub>2</sub>	A3	A4	A5	A6
1	0.199322	0.002452	-0.081722	-0.003181	-0.000569	0.010554
2	0.460116	-0.066706	-0.120368	0.002554	-0.001168	0.015310
3	2.567918	-0.485771	-0.460969	0.023309	0.003067	0.054005
4	10.559480	-2.613615	-1.550354	0.219032	0.043157	0.107953
5	56.535180	-22.67026	11.456380	2.512294	1.195645	-2.908978
6	4.556402	-0.988243	-0.605158	0.056484	0.006011	0.069641
7	2.413270	-0.407942	-0.546100	0.019668	0.010303	0.055666
8	3.523753	-1.456466	0.436200	0.146622	-0.002814	-0.073248
9	23.166410	-7.684319	0.816435	0.768879	0.270188	-0.473434
10	1.890447	-0.937951	0.448627	0.131430	0.067787	-0.151218

Table A.5: Coefficients for the correlations of the band absorption coefficient of a  $H_2O$ -CO<sub>2</sub> mixture with  $M_r$ =1/8.

Table A.6: Coefficients for the correlations of the band absorption coefficient of a H<sub>2</sub>O-CO<sub>2</sub> mixture with  $M_r=1/4$ .

BAND NO.	A1	A2	A3	A4	A5	A6
1	0.331540	0.001619	-0.144560	-0.004914	-0.000999	0.018540
2	0.547611	-0.083501	-0.144379	0.003801	-0.001309	0.017803
3	4.245958	-0.842435	-0.680102	0.043555	0.008076	0.076821
4	11.202300	-2.576854	-1.919555	0.201280	0.043926	0.158788
5	52.426210	-21.00060	10.501360	2.330265	1.110232	-2.685676
6	6.345440	-1.337306	-0.893243	0.074528	0.013760	0.099064
7	4.112496	-0.764805	-0.781350	0.042099	0.022972	0.073043
8	5.181861	-1.991517	0.533868	0.189612	-0.002467	-0.088538
9	22.653980	-7.623501	1.042302	0.765537	0.263117	-0.494163
10	2.620030	-1.075018	0.359544	0.145443	0.103480	-0.170703

BAND NO.	<b>A</b> 1	A <sub>2</sub>	A3	A4	A5	A6
1	0.579222	-0.016965	-0.232978	-0.006102	-0.001557	0.029676
2	0.696623	-0.116735	-0.171070	0.006394	-0.001303	0.020184
3	6.660610	-1.357929	-0.986873	0.072886	0.016014	0.108338
4	12.020590	-2.498614	-2.424063	0.173683	0.045697	0.228792
5	45.966350	-18.37492	9.002218	2.043978	0.976053	-2.335062
6	8.873031	-1.828428	-1.298180	0.099676	0.025613	0.140053
7	6.543768	-1.271468	-1.120598	0.073450	0.041902	0.098248
8	7.247368	-2.653061	0.647058	0.242334	-0.001979	-0.106229
9	21.397300	-7.354324	1.315303	0.743811	0.248349	-0.511823
10	3.663677	-1.243549	0.178492	0.160816	0.152501	-0.188653

Table A.7: Coefficients for the correlations of the band absorption coefficient of a H<sub>2</sub>O-CO<sub>2</sub> mixture with  $M_r=1/2$ .

Table A.8: Coefficients for the correlations of the band absorption coefficient of a H<sub>2</sub>O-CO<sub>2</sub> mixture with M<sub>r</sub>=1.

BAND NO.	A <sub>1</sub>	A <sub>2</sub>	A3	A4	A5	A6
1	0.919122	-0.050875	-0.339151	-0.006720	-0.002178	0.042970
2	0.877775	-0.158920	-0.197953	0.009788	-0.001119	0.022207
3	9.613162	-1.987588	-1.360774	0.108578	0.026032	0.146709
4	12.893730	-2.377743	-2.992425	0.138231	0.049245	0.307937
5	37.166590	-14.80333	6.976153	1.655044	0.794430	-1.860952
6	11.928440	-2.417743	-1.792236	0.129435	0.040327	0.190125
7	9.502207	-1.881765	-1.542546	0.110609	0.065159	0.130306
8	9.472530	-3.357394	0.751424	0.297754	-0.001391	-0.122498
9	19.349500	-6.853713	1.623699	0.701101	0.224327	-0.523703
10	4.952210	-1.433418	-0.075431	0.176454	0.210895	-0.204262

Table A.9: Coefficients for the correlations of the band absorption coefficient of a H<sub>2</sub>O-CO<sub>2</sub> mixture with M<sub>r</sub>=2.

BAND NO.	A <sub>1</sub>	A2	A3	A4	A5	A <sub>6</sub>
1	1.271382	-0.089230	-0.443173	-0.006974	-0.002755	0.055954
2	1.043090	-0.198014	-0.221590	0.013038	-0.000830	0.023742
3	12.533690	-2.609370	-1.731498	0.143698	0.036029	0.184815
4	13.721570	-2.273590	-3.464707	0.105218	0.055098	0.373611
5	27.080330	-10.72507	4.696161	1.212122	0.588806	-1.326135
6	14.929170	-2.993108	-2.282060	0.158181	0.054901	0.239899
7	12.418670	-2.479104	-1.965455	0.146590	0.088115	0.162958
8	11.438490	-3.970542	0.825736	0.345208	-0.000736	-0.134068
9	16.876780	-6.218208	1.945330	0.645129	0.192917	-0.530026
10	6.291047	-1.629235	-0.335575	0.191338	0.268061	-0.217563